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Theoretical aspects of the Fe_cNi_{1-c} Invar alloy

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We present first-principles coherent-potential-approximation calculations for the fcc FeNi alloy. We have found that this system is characterized by a competition between a low-spin (LS) and a high-spin (HS) state, and we have calculated this energy difference as a function of alloy concentration. For fcc Fe we find that several magnetic states are locally stable whereas for the FeNi alloys only one magnetic state is stable. In agreement with previous theories for explaining the Invar effect in the $Fe_{65}Ni_{35}$ alloy, we find that at this concentration the LS and HS states are very similar in energy. The calculated magnetic moment, equilibrium volume, and bulk modulus agree well with experimental data, and we predict that the Grüneisen constant exhibits an anomaly at a Ni concentration around 25%.

The Fe-Ni system displays many interesting properties and no doubt most of the attention has been focused on the Invar behavior of this alloy.[1] Since this almost 100 year old discovery, many more alloys and even some compounds have been found to have almost no thermal expansion, thus qualifying as Invar systems.[2] Another interesting aspect about the Fe_cNi_{1-c} alloys is the change of crystal structure from bcc for the Fe-rich alloys to fcc for the systems with larger Ni concentration. To complicate the situation further the magnetic moment for the iron-nickel alloy initially follows the Slater-Pauling curve in the bcc phase but right after the stabilization of the fcc structure the magnetic moment is first almost zero, and then with a further increase of the Ni concentration it increases sharply. At even higher Ni concentrations the moment again follows the Slater-Pauling curve. The change of the crystal structure and the complicated behavior of the magnetic moment at alloy concentrations corresponding to the Invar alloy have been speculated to be crucial aspects of the explanation of the invariant thermal expansion.

A number of theoretical models for describing the Invar effect have been proposed.[2] One of the earlier phenomenological models is due to Weiss[3] who introduced the so-called 2γ state model, where two magnetically ordered states, one ferromagnetic and one antiferromagnetic, have different equilibrium volumes but very similar energy. The thermal excitation of the two-component system, including excitations to the low-volume state, was thus proposed to compensate the anharmonic effect of the lattice vibrations, thus explaining the Invar effect. Later theoretical work, based on *ab initio* band structure calculations, has in general confirmed this picture,[4–14] although the type of magnetic order for the low-volume state is still under discussion. These calculations led to the following model: In pure fcc Fe a low-spin (or paramagnetic) state, with a relatively low equilibrium volume, is a locally stable state, while at expanded volumes a high-spin state is stable. The resulting binding energy curve as a function of volume is formed by the two crossing branches corresponding to the low-spin (LS) and the high-spin (HS) states. As the Ni concentration increases, the difference in energy between the LS and the HS states decreases, and at a certain concentration the HS state becomes stable. Based on this model Moruzzi[9–11] gave a qualitative explanation of the Invar effect and a number of other properties of Invar alloys.

Although a rather large body of theoretical data has been accumulated for the Fe_cNi_{1-c} alloys, no *ab initio* calculations have been presented describing the variation of the total energy of the paramagnetic (PM) and ferromagnetic (FM) states as a function of alloy concentration. The concentration dependence of the PM-FM energy difference was, for example, estimated by a linear interpolation between the values obtained for pure Fe and Co.[10] The lack of first-principles calculations of the PM-FM energy difference of these alloys is most probably due to the fact that treating a random alloy theoretically is not an easy task. In most of the previous theoretical treatments one has instead replaced the alloy with a perfectly ordered compound, e.g., Fe_3Ni.[10,12–14] Although the results presented in Refs. 10, 12–14 seem to reproduce much of the experimental data for the Fe_3Ni compound, one worry with this approach is the neglect of disorder. Also, by this approach one is faced with the obvious drawback of being able to treat only systems with specific Fe and Ni concentrations (unless a huge supercell is considered).

Despite the above mentioned difficulty in describing the electronic properties of random alloys, a num-

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ber of calculations which considered a random Fe-Ni alloy have been performed recently in the framework of the Korringa-Kohn-Rostoker coherent-potential-approximation (KKR-CPA) method. For example, Johnson *et al.*[15,16] have calculated the electronic structure of the Invar $Fe_{65}Ni_{35}$ alloy and determined the magnetic moment as a function of concentration and volume. Also, Akai and Dederichs[17] have calculated total energies of the random fcc FeNi alloy in the concentration interval close to the Invar region and reported the possibility of the existence of a state with local moment disorder (LMD). Therefore, it is very desirable to perform a CPA total energy calculation for the random Fe_cNi_{1-c} alloy over the complete concentration interval $0 \leq c \leq 1$, since only by doing this can one calculate the ground state properties without having to rely on too crude approximations for the alloy state, and thus investigate the validity of the Weiss model (modified so that one replaces the antiferromagnetic state with a nonmagnetic or low-spin state). Another motivation for the present study is the above mentioned, intriguing behavior of the equilibrium ground state thermodynamic and magnetic properties as a function of alloy concentration.

In this work we thus present results of first-principles local-spin-density (LSD) calculations of the total energy, magnetic moment, and thermodynamic ground state properties of the fcc random Fe_cNi_{1-c} ($0 \leq c \leq 1$) alloy obtained by the fully self-consistent all-electron, scalar-relativistic, linear muffin-tin orbital (LMTO) method.[18–23] The disorder was treated in the framework of the single-site CPA. All calculations, including those for the pure elements, were performed by the Green's function technique rather than by diagonalizing the corresponding Hamiltonian. Even though charge transfer effects are small in the Fe-Ni system, their influence was taken into account by the correction term to the Madelung potential and energy, as proposed in Refs. 24, 25. The complete method is described in detail in Ref. 26 with the exception that here we calculate the potential functions directly from the solutions to the Schrödinger equation at each energy on the contour without the usual expansion in terms of potential parameters.

We note that in order to calculate accurate total energies we had to use the fixed spin moment (FSM) method[8,9] which is essential for regions where there is a transition from a PM to a FM state, for reasons which we will explain below. We did not consider the possibility of an antiferromagnetic state or a LMD state in this work. Moreover, we employed the Vosko-Wilk-Nusair parametrization[27] for the exchange-correlation energy density and potential, and the basis set included s, p, and d orbitals only. The k-space integral was calculated in the 1/48th part of the Brillouin zone at 240 k points of the fcc lattice. All energy integrals were evaluated on a semicircular contour in the complex energy plane by means of 16 energy points. The convergence criteria for the total energy was 0.001 mRy. In order to determine equilibrium ground state parameters as a function of volume we used an exponential function fit, proposed by Moruzzi *et al.*[28] The minimization of the total energy as a function of magnetic moment for a fixed volume was done by a cubic spline interpolation, except for the volumes where the magnetic moment corresponding to the lowest total energy is small. For these volumes we employed a Landau expansion of the energy $E_{\rm tot}$ in even powers of magnetic moment M (up to the fourth power),

$$E_{\rm tot}(M,V) = E_{\rm tot}(0,V) + \alpha(V)M^2 + \beta(V)M^4, \quad (1)$$

where $E_{\rm tot}(0,V), \alpha(V)$, and $\beta(V)$ are volume-dependent parameters which are determined by fitting (least squares minimization) Eq. (1) to the values of $E_{\rm tot}$ calculated for different (small) magnetic moments (keeping the volume V fixed). In Ref. 29 it was shown that this approach gives the correct volume dependence of the magnetic moment close to the PM-FM transition.

First, we describe the results of the FSM calculations for a few selected alloy concentrations. In Fig. 1 we show

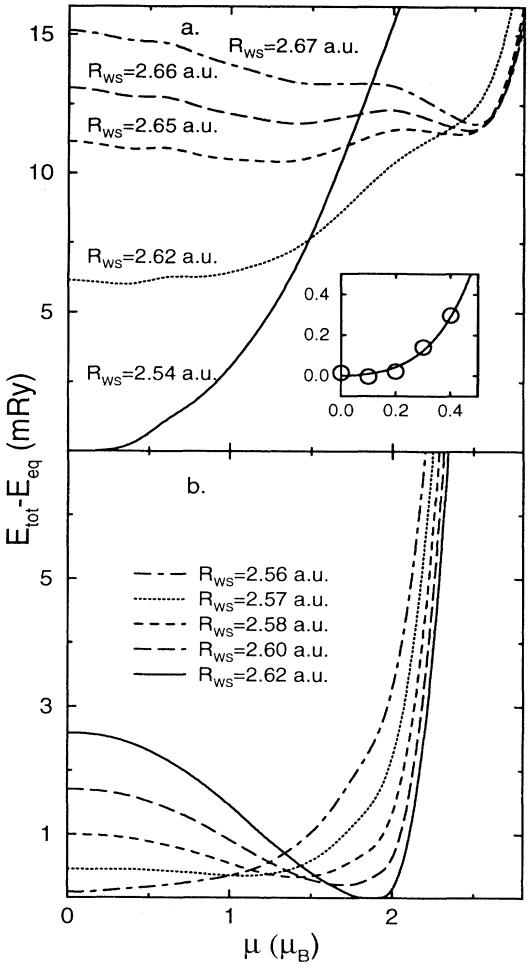

FIG. 1. Total energy (relative to the equilibrium energy) as a function of constrained magnetic moments for pure fcc Fe (a) and fcc $Fe_{74}Ni_{26}$ alloy (b) at different Wigner-Seitz radii $R_{\rm WS}$. The inset in panel (a) shows the curve for pure fcc Fe at $R_{\rm WS}$=2.54 a.u., and has the same axis labels as the main figure. In the inset calculated values of the total energy are shown by the open circles, while the solid drawn line represents a least squares fit by means of Eq. (1).

the total energy as a function of the constrained magnetic moment (Lagrangian multiplier) for pure Fe and the random $Fe_{74}Ni_{26}$ alloy, calculated at several lattice constants. It is seen in Fig. 1(a) that for pure fcc Fe the energy has local minima at several magnetic moments, depending on the volume. This behavior is understandable from the shape of the canonical state density for the fcc lattice,[6,7] and has already been found in the previous studies of the binding energy of fcc Fe.[8,10] Note that this complicated behavior of the total energy makes the convergence of the conventional floating (not fixed) spin moment calculations extremely poor, and we have found that the only way to obtain a reliable total energy of the present system is to apply the fixed spin moment method.

The observed dependence of the energy on the magnetic moment and the volume is in agreement with the results of Refs. 8, 10, where also three types of solutions [paramagnetic (PM), low spin (LS), and high spin (HS)] were reported. However, unlike previous studies we have found that the state with a small magnetic moment of about $0.2\mu_B$ gives the lowest total energy for fcc Fe at Wigner-Seitz radii between 2.63 a.u. and 2.565 a.u., although the energy difference between this state and the PM state is extremely small (of order 0.01 mRy) and is almost the same as the convergence criteria for our calculations. Therefore, it is essential to use the Landau expansion (1) in this volume interval. By doing so we can partially remove the numerical inaccuracy of our calculated energies. As an example of how well this fitting works we show in the inset in Fig. 1(a) the calculated and fitted energies of fcc Fe at a Wigner-Seitz radius of 2.54 a.u.

We find that the transition from the FM state to the PM state is continuous, exhibits a square-root singularity [see Fig. 2(a)] predicted theoretically in Ref. 29, and takes place at a volume which is slightly larger than the equilibrium volume. So in agreement with previous studies the ground state of pure fcc Fe is found to be paramagnetic (remember that the antiferromagnetic solution was not considered in this work). Moreover, since the energy difference between the FM and the PM solutions is extremely small for Wigner-Seitz radii below 2.63 a.u., in the following discussion we will refer to the state with magnetic moment in the range $0 < \mu < 0.5\mu_B$ as the low-spin (LS) state, while we will refer to the state with magnetic moment in the interval $0.7\mu_B < \mu < 1.55\mu_B$ as the intermediate-spin (IS) state, and the state with a magnetic moment $2.0\mu_B < \mu$ as the high-spin (HS) state. As the volume is increased from the equilibrium value one observes in Fig. 2 first-order transitions from the LS state over the IS state to the HS state. The first-order character of these LS-IS-HS transitions results in the existence of three crossing branches of the binding energy curve [see Fig. 2(b)] which means that the corresponding first derivative has discontinuities at the crossing points. Note from Fig. 2(b) that the energy difference between the LS and the IS states is also very small.

Next, we show that the behavior of the total energy and the magnetic moment as a function of volume is changed significantly in the case of a random alloy ($Fe_{74}Ni_{26}$). First, one observes in Fig. 1(b) that for the

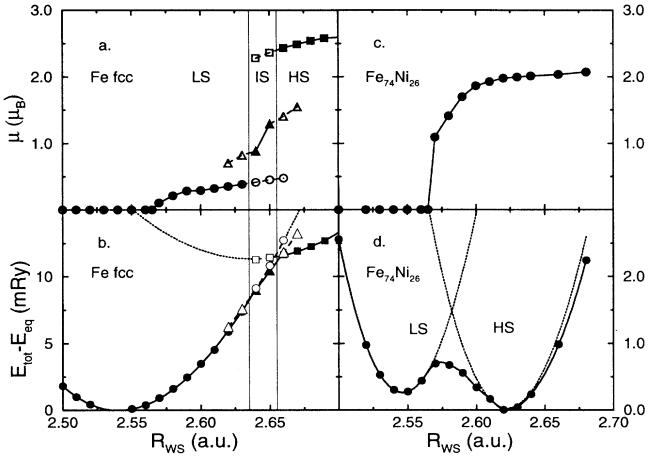

FIG. 2. Average magnetic moment [(a) and (c)] and total energy (relative to the equilibrium energy) [(b) and (d)] as a function of Wigner-Seitz radii R_{WS} for pure fcc Fe [(a) and (b)] and fcc $Fe_{74}Ni_{26}$ alloy [(c) and (d)]. Solid drawn lines with solid symbols correspond to the global minimum of energy as a function of constrained magnetic moment, dashed lines with open symbols represent a local minimum, and dotted lines are extrapolations of the corresponding branches of the binding energy curve to volumes where these states are not stable even locally. In (a) and (b) circles are used for the low-spin state, triangles denote the intermediate-spin state, and squares are for the high-spin state.

fcc $Fe_{74}Ni_{26}$ alloy there is only one (global) minimum; at zero magnetic moment or at a finite moment, depending on volume. Metamagnetic states do not occur, due to the smearing of the state density in the alloy by the disorder. This results in a continuous change of the average magnetic moment as a function of volume [see Fig. 2(c)] with the square-root singularity at the PM-FM transition (found at a Wigner-Seitz radius of 2.565 a.u.), as expected from the analysis presented in Ref. 29. Second, the difference in energy between the LS and the HS states decreases when the concentration of Ni increases, and is almost zero for the $Fe_{74}Ni_{26}$ alloy, as shown in Fig. 2(d). The behavior of the binding energy curve is also different [Fig. 2(d)] since there is no crossing of different branches any more, as was the case for pure fcc iron. In Fig. 2(d) we also display two energy curves (dotted lines) where the moment was fixed to be either zero or to the value corresponding to the energy minimum of the HS state ($\mu = 1.98\mu_B$). Notice that at volumes in between the LS and HS equilibrium volumes the ground state energy is significantly lower than the two dotted curves in Fig. 2(d). Notice also that in Figs. 2(b) and 2(d) we have made use of three different ways to represent the total energy curves: solid drawn lines with solid symbols, dashed lines with open symbols, and dotted lines. The solid drawn curve represents the global minimum whereas the dashed curve represents a local minimum. The dotted curve is simply an extrapolation of the energies for the corresponding states and for this curve the energy can always be lowered even by an infinitely small modification of the magnetic moment (in contrast to the dashed, metastable curve).

The results of the FeNi alloy are important when analyzing the model used by Moroni and Jarlborg[14] for calculating the thermal expansion coefficient of an ordered Fe_3Ni compound (simulating the Invar alloy). In their model Moroni and Jarlborg considered only thermal excitations which conserve the volume, e.g., from the high-spin state to the low-spin state. However, the present CPA calculation shows that for Fe_cNi_{1-c} alloys this mechanism is not possible, since for volumes where the high-spin state has the lowest energy the low-spin state is not even locally stable [Figs. 1(b) and 2(d)]. The theory provided by Mohn *et al.*,[12] which considers a Landau-Ginzburg expansion of the total energy seems to avoid such difficulties.

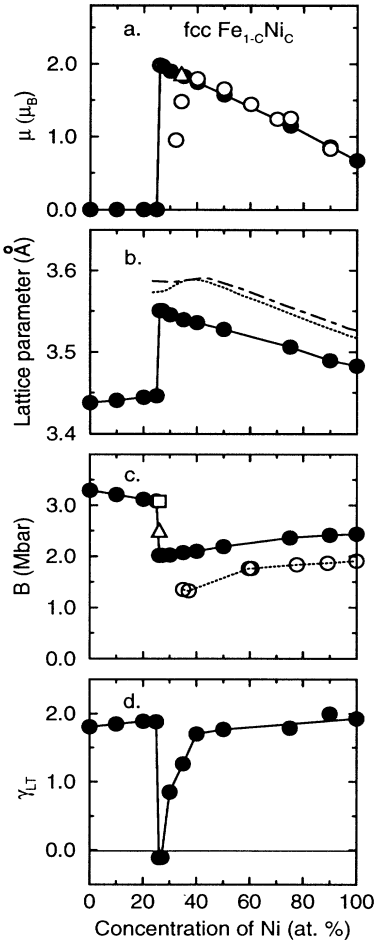

FIG. 3. Average magnetic moment (a), lattice parameter (b), bulk modulus (c), and low-temperature Grüneisen constant (d) as a function of alloy concentration of fcc $Fe_{1-c}Ni_c$. Solid circles are calculated results. Bulk moduli for $Fe_{74}Ni_{26}$ obtained for the LS (open square) and HS (open triangle) artificial binding energy curves [dotted lines in Fig. 2(d)] are presented in (c). The experimental data for the average magnetic moment (open circles at room temperature, open triangle at $T = 77$ K, Ref. 30), lattice parameter (dotted line at room temperature, dot-dashed line at $T = 473$ K, Ref. 31), and bulk modulus (open circles at $T = 4.2$ K, Ref. 32) are also shown.

It is also obvious that the described behavior of the binding energy curve for the fcc FeNi alloy should lead to anomalies in the ground state magnetic and thermodynamic properties. In Fig. 3 we demonstrate that this is the case, by presenting the calculated and experimental data for the magnetic moment, equilibrium volume, bulk modulus, and Grüneisen constant as a function of alloy concentration. The calculated points were extracted at the volume where the total energy is lowest. Notice that the experimental data are only shown for the fcc structure, which at room temperature is stable in the Ni concentration range 65–100 %, while the theoretical results are given for the fcc alloy in the complete concentration interval (we did not consider the bcc alloy in this work). Starting with the magnetic moment it is clear from Fig. 3(a) that in the Ni-rich region where the HS state is stable both the theoretical and experimental curves follow the Slater-Pauling curve and the agreement between theory and experiment is excellent. In the iron-rich region there may exist a very small local moment on the Fe and the Ni atoms (for the alloy with 25% Ni they are $0.0008\mu_B$ and $-0.0023\mu_B$ for the Fe and Ni atoms, respectively). For all Fe-rich alloys we find that the Fe and Ni moments are directed antiparallel and that the net moment is exactly zero. For a Ni concentration of $\sim 26\%$ we calculate a first-order magnetic phase transition from a paramagnetic to a ferromagnetic state, because at this concentration the HS state becomes more stable than the LS state as we show in Fig. 4 where the energy difference between the LS and HS states is plotted as a function of alloy concentration. Experiments at room temperature show, however, a second-order transition, from a HS state to a state with zero average magnetic moment, at a concentration of $\sim 35\%$ of Ni. We will return to this disagreement later.

Next we observe that, in agreement with expectations, for calculations based on the LSD approximation, the equilibrium volume is underestimated and the bulk mod-

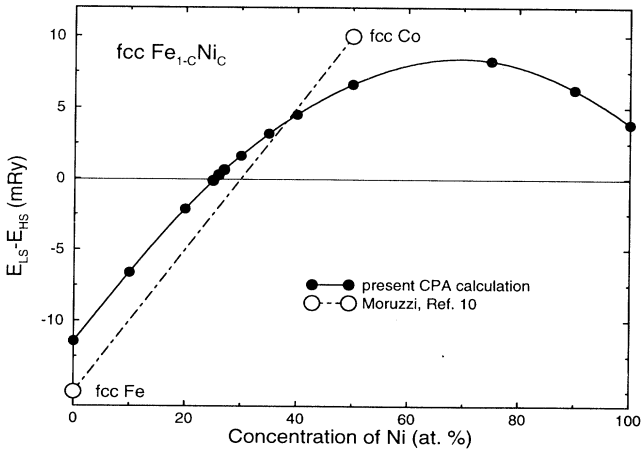

FIG. 4. Energy difference between the low-spin and the high-spin states in FeNi alloys as a function of Ni concentration. Solid line with solid circles: calculated results. Dot-dashed line with open circles: the linear interpolation between the points for the pure fcc Fe and Co used in Ref. 10.

ulus is overestimated. However, the trends displayed by these properties as a function of alloy concentration are described very well by our CPA theory [see Figs. 3(b) and (c)]. Both the lattice parameter and the bulk modulus exhibit a linear behavior as a function of concentration, except for the alloy concentration where there is a transition from the LS to the HS state. Due to magnetovolume effects, the HS state is expected to have a larger equilibrium volume than the LS state, in agreement with the calculations of Fig. 3(b). The decrease of the bulk modulus at the LS $\rightarrow$ HS transition can partly be explained by magnetovolume effects [compare the open square and open triangle in Fig. 3(c)]. However, the change of the magnetic moment of the HS state as a function of volume [Fig. 2(d)] decreases the curvature of the HS energy curve, which lowers the bulk modulus further. To illustrate this effect we show in Fig. 3(c) the bulk modulus of the random $Fe_{74}Ni_{26}$ alloy evaluated from the fixed spin moment calculation in Fig. 2(d) (dotted curve with a moment fixed to $1.98\mu_B$). The so-obtained bulk modulus is considerably higher than the value obtained from the ground state energy curve.

In Fig. 3(d) we show the concentration dependence of the low-temperature Grüneisen constant, which enters the Debye-Grüneisen model for the calculation of the thermal expansion[28] and is defined as

$$\gamma_{\mathrm{LT}} = -1 - \frac{V}{2}\frac{\partial^2 P/\partial V^2}{\partial P/\partial V}, \tag{2}$$

where P is the pressure and V is the volume. Notice that around the concentration where the LS to HS transition occurs the Grüneisen constant is highly anomalous. The origin of this anomaly lies in the second-order character of the transition from the LS to HS state. As a result of the rapid, but continuous change of the magnetic moment, the increase in the energy is anomalously small when the volume is decreased from the HS equilibrium volume [see Fig. 2(d)]. Such a behavior of the binding energy leads to a small, and even a negative, value of the low-temperature Grüneisen constant. This in turn, according to the Debye-Grüneisen model, should lead to an anomalous negative thermal expansion at temperatures well below room temperature. Note that a two-state model based on conventional HS and LS state energy curves [for instance, with the same shape as the two dotted curves in Fig. 2(d)] fails to explain the low-temperature behavior of the thermal expansion coefficient since in this case the low-temperature equilibrium properties are determined by either the LS or the HS solutions only. As a result the theoretical thermal expansion coefficient is always positive at low temperatures,[10,14] in contrast to the experimental observation that it is negative.[2]

We now return to the alloy concentration where the transition from the LS state to the HS state occurs, and focus on the disagreement between the theoretical (26%) and experimental (35%) values. One possibility for this is of course that it is the usual discrepancy between a first-principles, parameter-free calculation and reality. However, there might exist a different reason for the disagreement. In connection to this let us first analyze the results presented by Moruzzi, who, when studying the Invar problem in his LS-HS model,[10] arrived at the conclusion that the energy difference between the LS and the HS solutions should be zero at about 35% of Ni, in agreement with experimental data. However, he used a linear interpolation between the values obtained for pure Fe and Co in order to estimate the transition concentration of the alloy. On the other hand, one can see in Fig. 4 that the concentration dependence of the LS-HS energy difference, as obtained by our CPA calculations, has a parabolic shape. This is to be expected from simple band filling arguments of a rectangular density of states model, proposed by Friedel.[33] Here the d electrons contribute to the bonding energy with an amount $U_d^{\mathrm{bond,PM}} = -(W/20)N_d(10 - N_d)$, where W is the alloy bandwidth. This term has a quadratic dependence on the number of d electrons, N_d. Similarly, in the model of saturated ferromagnetism, where a complete filling of the majority spin band is assumed, the bonding energy can be written as $U_d^{\mathrm{bond,FM}} = -(W/10)N_d^{\mathrm{down}}(5 - N_d^{\mathrm{down}})$, and this term also has a parabolic dependence on the number of spin-down electrons, N_d^{down}. The difference $U_d^{\mathrm{bond,PM}} - U_d^{\mathrm{bond,FM}}$ is also a parabolic function of the band filling, in agreement with our first-principle calculations (Fig. 4). The excellent result of Moruzzi, concerning the concentration for the occurrence of the LS $\rightarrow$ HS transition, thus seems to be somewhat fortuitous.

Let us now investigate some possible explanations for the observed disagreement between theory and experiment. We first point out that we do not expect that short-range order effects are responsible, because in the Fe_3Ni compound, which corresponds to maximal short-range order, the HS solution is already more stable than the LS one.[10,12–14] Instead the reason might be due to the fact that the experimental values of the lattice parameters and the average magnetic moments, presented in Fig. 3, were obtained at room temperature, whereas our calculations were performed at zero temperature. To investigate this hypothesis we compare in Figs. 3(a) and 3(b) some experimental data of the lattice constant and magnetic moment at different temperatures. Notice that concerning the lattice constant the transition is shifting to higher Ni concentration as the temperature is increased. Also, at low-temperature the magnetic moment of the $Fe_{64}Ni_{36}$ alloy is considerably higher than the value reported at room temperature and the low-temperature value is actually in very good agreement with our calculations. This strong temperature dependence of the magnetism in the Ni concentration range around 35% is to be expected, since the Curie temperature drops to low values at these concentrations.

The experimental data in Fig. 3(a), when considering also the low-temperature value of the $Fe_{64}Ni_{36}$ alloy, may indicate that the LS $\rightarrow$ HS transition is first order, in agreement with our calculations. Also, the critical concentration at which this transition occurs is moved to lower Ni concentrations when the temperature is lowered and is approaching our calculated value. As the temperature increases, the metastable states can be thermally populated, and the transition from paramagnetism to ferromagnetism becomes less abrupt, and may even become of second order. We thus propose that the observed

disagreement between theory and experiment concerning the LS to HS state is due to temperature effects. It is also possible that some other phases are present in the Invar alloys. For example, Akai and Dederichs[17] reported the possibility of the existence of a state with local moment disorder (LMD) which in their calculations was found to be more stable compared to the FM state at the Invar concentration. In this case one should expect even more complicated behavior of the binding energy curve, and since the equilibrium volume for the LMD state lies between that of the LS and that of the HS states,[17] the less sharp transition of, say, the lattice parameter can be expected.

In conclusion we have reproduced a number of experimental data for FeNi alloys, such as magnetic moment, equilibrium volume, and bulk modulus. The transition from a LS state for the Fe-rich alloys to a HS state for the Ni-rich alloys is calculated to take place at a Ni concentration of 26% which is in fair agreement with the experimental concentration of 35%. We argue that the discrepancy might be due to thermal effects. The LS $\rightarrow$ HS transition results in an anomalous Grüneisen constant at the critcal concentration and this in turn should result in a small negative thermal expansion at low temperatures, in agreement with experiment. The magnetism in fcc Fe is found to be characterized by several metamagnetic states whereas for the FeNi alloy only one state (LS, IS, or HS) is stable.

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[1] C. E. Guillaume, C. R. Acad. Sci. **125**, 235 (1897).
[2] E. F. Wasserman, in *Ferromagnetic Materials*, edited by K. H. J. Buschow and E. P. Wohlfarth (North-Holland, Amsterdam, 1990), Vol. 5, p. 237.
[3] R. J. Weiss, Proc. R. Soc. London **82**, 281 (1963).
[4] J. Madsen, O. K. Andersen, U. K. Poulsen, and O. Jepsen, in *Magnetism and Magnetic Materials—1975 (Philadelphia)*, Proceedings of the 21st Annual Conference on Magnetism and Magnetic Materials, edited by J. J. Becker, G. H. Lander, and J. J. Rhyne, AIP Conf. Proc. No. 29 (AIP, New York, 1976), p. 327.
[5] U. K. Poulsen, J. Kollar, and O. K. Andersen, J. Phys. F **6**, L241 (1976).
[6] O. K. Andersen, J. Madsen, U. K. Poulsen, O. Jepsen, and J. Kollar, Physica B **86-88**, 249 (1977).
[7] D. M. Roy and D. G. Pettifor, J. Phys. F **7**, L183 (1977).
[8] V. L. Moruzzi, P. M. Marcus, K. Schwarz, and P. Mohn, Phys. Rev. B **34**, 1784 (1986).
[9] V. L. Moruzzi, Physica B **161**, 99 (1989).
[10] V. L. Moruzzi, Phys. Rev. B **41**, 6939 (1990).
[11] V. L. Moruzzi, Solid State Commun. **83**, 739 (1992).
[12] P. Mohn, K. Schwarz, and D. Wagner, Phys. Rev. B **43**, 3318 (1991).
[13] P. Entel, E. Hoffmann, P. Mohn, K. Schwarz, and V. L. Moruzzi, Phys. Rev. B **47**, 8706 (1993).
[14] E. G. Moroni and T. Jarlborg, Phys. Rev. B **41**, 9600 (1990).
[15] D. D. Johnson, F. J. Pinski, and G. M. Stocks, J. Appl. Phys. **57**, 3018 (1985).
[16] D. D. Johnson, F. J. Pinski, and J. B. Staunton, J. Appl. Phys. **61**, 3715 (1987).
[17] H. Akai and P. H. Dederichs, Phys. Rev. B **47**, 8739 (1993).
[18] O. K. Andersen, Phys. Rev. B **12**, 3060 (1975).
[19] O. Gunnarsson, O. Jepsen, and O. K. Andersen, Phys. Rev. B **27**, 7144 (1983).
[20] H. L. Skriver, *The LMTO Method* (Springer-Verlag, Berlin, 1984).
[21] O. K. Andersen and O. Jepsen, Phys. Rev. Lett. **53**, 2571 (1984).
[22] O. K. Andersen, O. Jepsen, and D. Glötzel, in *Highlights of Condensed-Matter Theory*, edited by F. Bassani, F. Fumi, and M. P. Tosi (North-Holland, New York, 1985).
[23] O. K. Andersen, Z. Pawlowska, and O. Jepsen, Phys. Rev. B **34**, 5253 (1986).
[24] I. A. Abrikosov, Yu. H. Vekilov, P. A. Korzhavyi, A. V. Ruban, and L. E. Shilkrot, Solid State Commun. **83**, 867 (1992).
[25] P. A. Korzhavyi, A. V. Ruban, S. I. Simak, and Yu. Kh. Vekilov, Phys. Rev. B **49**, 14 229 (1994).
[26] A. I. Abrikosov and H. L. Skriver, Phys. Rev. B **47**, 16 532 (1993).
[27] S. H. Vosko, L. Wilk, and M. Nusair, Can. J. Phys. **58**, 1200 (1908).
[28] V. L. Moruzzi, J. F. Janak, and K. Schwarz, Phys. Rev. B **37**, 790 (1988).
[29] V. L. Moruzzi, Phys. Rev. Lett. **57**, 2211 (1986).
[30] Landolt-Börnstein, *Numerical Data and Functional Relationship in Science and Technology*, New Series (Springer-Verlag, Berlin, 1986), Vol. III/19a, p. 142.
[31] W. B. Pearson, *A Handbook of Lattice Spacing and Structure of Metals and Alloys* (Pergamon Press, London, 1967).
[32] D. I. Bower, E. Claridge, and I. S. T. Tsong, Phys. Status Solidi **29**, 617 (1968).
[33] J. Friedel, Ann. Phys. (N.Y.) **1**, 257 (1976).